Precomputed wind field database for fast atmospheric dispersion calculation: modelling of low frequency effects with triple decomposition

22nd International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes

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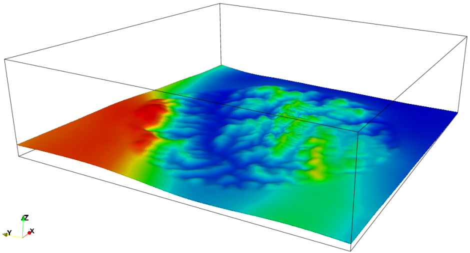
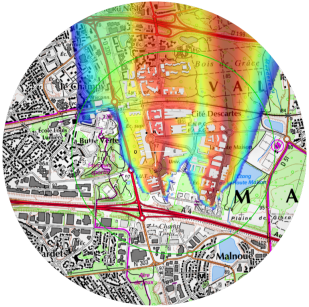
June 13, 2024

CFD for atmospheric flows @ EDF and CEREA

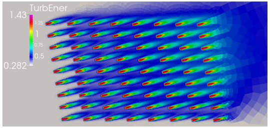
Using the open-source CFD solver code_saturne (www.code-saturne.org)



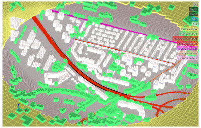
Wind potential estimates on complex terrain

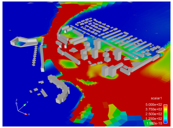


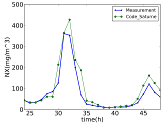
Air quality map in real time



Wake effects on an offshore wind farm (WRAPP)



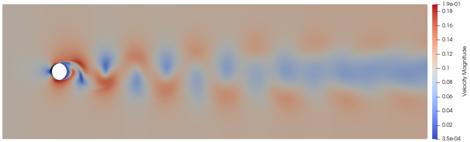




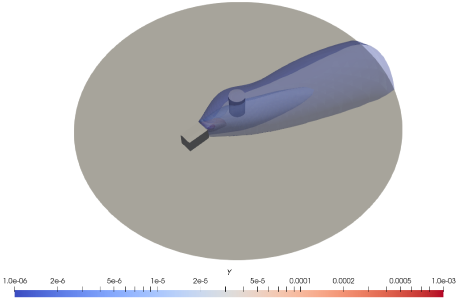
Air quality (Toulouse, Marseille, Villiers-sur-Marne, ...)

cerea
École des Ponts ParisTech
code_saturne

Motivation



Inner low-frequency oscillations, e.g.: Von Kármán instabilities.



Outer low-frequency oscillations, e.g.: wind direction oscillations, meandering in case of low-wind.

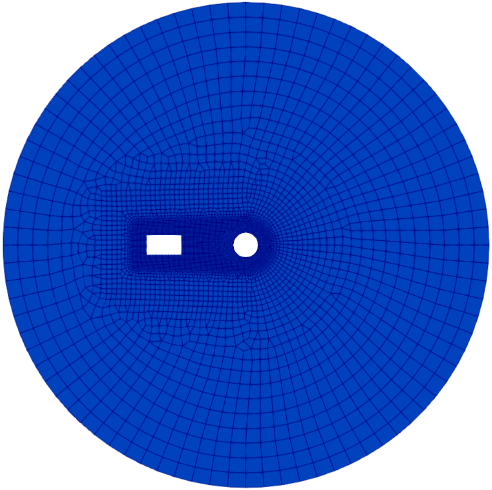
Objective of the presentation

Propose a diffusion model, to reconstruct the part of the dispersion lost during a frozen-field computation.

Overview

Methodology presentation on a toy model

- CFD for atmospheric flows
  - Local microscale: $\approx 2\,\mathrm{km}$ diameter.
  - Atmospheric boundary layer: $\approx 200\,\mathrm{m}$ high.
  - Taking into account buildings and relief.
- Mesh with code_saturne_atmo_mesher scripts based on open-source platform SALOME
  - Buildings zone refinement : $1.5\,\mathrm{m}$



Mesh horizontal slice ($z = 10\,\mathrm{m}$)

Setup of equations

Reynolds-averaged $\overline{(\cdot)}$ Navier-Stokes equations

$$\frac{\partial \rho}{\partial t} + \text{div}\,(\rho \underline{\overline{u}}) = 0,$$

$$\frac{\partial (\rho \underline{\overline{u}})}{\partial t} + \underline{\text{div}}\,(\underline{\overline{u}} \otimes \rho \underline{\overline{u}}) = -\underline{\nabla} \overline{p} + \underline{\text{div}}\left(\underline{\underline{\tau}} - \rho \underline{\underline{R}}\right) + \rho \underline{g},$$

$$C_p \left(\frac{\partial (\rho \overline{\theta})}{\partial t} + \text{div}\,(\overline{\theta} \rho \underline{\overline{u}}) \right) = \text{div}\,\left(\lambda \underline{\nabla} \overline{\theta} - \rho C_p \overline{\theta' \underline{u}'}\right),$$

with $k - \epsilon$ closure

$$\frac{\partial (\rho k)}{\partial t} + \text{div}\,(k \rho \underline{\overline{u}}) = \text{div}\,\left(\underline{Q}_k\right) + \rho\,(\mathcal{P} - \epsilon + \mathcal{G}),$$

$$\frac{\partial (\rho \epsilon)}{\partial t} + \text{div}\,(\epsilon \rho \underline{\overline{u}}) = \text{div}\,\left(\underline{Q}_\epsilon\right) + \rho \frac{\epsilon}{k}\,(C_{\epsilon_1} \mathcal{P} - C_{\epsilon_2} \epsilon + C_{\epsilon_3} \mathcal{G}),$$

Boundary conditions: *Monin and Obukhov 1954* profiles

Reynolds decomposition

$$f = \overline{f} + f'$$

$\overline{f}$ is an ensemble average of f

Under anelastic or Boussinesq approximation on density variation, steady equations rescale with velocity.
This similarity can be used to reduce the size of a precomputed data base.

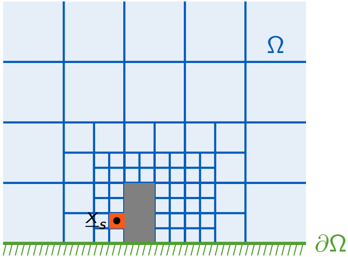
$$\underline{\overline{u}} = \mathcal{U} \times \underline{\overline{u}}^{\propto}$$

$\underline{\overline{u}}^{\propto}$ is the rescaled velocity resolved in the dynamic basis.

Building of an Atmospheric Transfert Coefficient (ATC) basis for pollutant dispersion

Transport equation of a passive scalar (concentration $\overline{C} = \rho\overline{Y}$, $\overline{Y}$ is the mass fraction)

$$\frac{\partial \rho \overline{Y}}{\partial t} + \text{div}\left(Y\rho\underline{\overline{u}}\right) - \text{div}\left(\underbrace{K\underline{\nabla}\overline{Y} - \rho\overline{Y'\underline{u}'}}_{\underline{Q}_Y}\right) = ST_Y$$



ATC definition:

$$ATC = \frac{\rho\overline{Y}_{simu}}{\dot{M}_Y} = \rho\overline{Y}_{simu} \quad \text{if } \dot{M}_Y = 1 \text{ kg/s (unitary mass flow rate)}$$

Obtention of ATC map for **volume emission**:

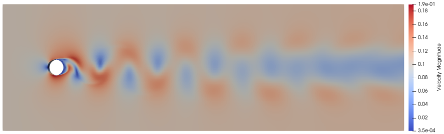
- if $\int_\Omega ST_Y \mathrm{d}\Omega = 1$ kg/s
- by defining $\overline{Y}^\propto = \mathcal{U}\overline{Y}$ and $ATC^\propto = \mathcal{U}ATC$

the steady transport equation becomes

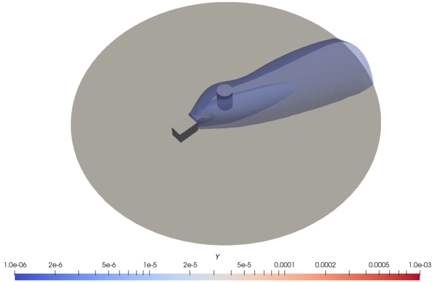
$$\text{div}\left(\overline{Y}^\propto \rho\underline{\overline{u}}^\propto\right) - \text{div}\left(\underline{Q}_Y\right) = \frac{1_{x\in\text{Volume emission}}}{\text{Volume emission}} \Leftrightarrow \text{div}\left(ATC^\propto\underline{\overline{u}}^\propto\right) - \text{div}\left(\underline{Q}_Y\right) = \frac{1_{x\in\text{Volume emission}}}{\text{Volume emission}}$$

What about low-frequency fluctuations?

- We store *steady* fields in our databases
- We need to reconstruct the dispersion "lost" in low-frequency instationnarities



Inner low-frequency oscillations, e.g.: Von Kármán instabilities.



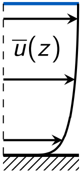
Outer low-frequency oscillations, e.g.: wind direction oscillations, meandering in case of low-wind.

Another motivation: harmonizing turbulence models

Apparent paradox for turbulent anisotropic ratio

Atmospheric surface layer:

$$\tau_{xz} = \rho u_\star^2 = -\rho \overline{u' w'}$$



$$k \approx \frac{u_\star^2}{\sqrt{C_\mu}} \quad \text{and} \quad \frac{|\overline{u' w'}|}{k} = \sqrt{C_\mu}$$

Reynolds averaging *versus Time averaging* (see e.g., *Richards and Norris 2011*, *Inagaki and Kanda 2010*)

$$\frac{\overline{u' w'}}{k} = \sqrt{C_\mu} \quad \textit{versus} \quad \frac{\frac{1}{T}\int_0^T u' w'}{\frac{1}{T}\int_0^T \frac{1}{2} u'_i u'_i}$$

"Pure" turbulence *Launder, Spalding, et al. 1972*

$$\sqrt{C_\mu} = \sqrt{0.09} = 0.3$$

Atmospheric flows *Duynkerke 1988*

$$\sqrt{C_\mu} = 0.18$$

Proposed methodology based on triple decomposition

- Unsteady RANS equations: fields are evolving with time.
- Reynolds decomposition :

$$\underline{u}(t) = \overline{\underline{u}}(t) + \underline{u}'(t)$$

- Time-average operator :

$$\langle f \rangle \equiv \lim_{T \to +\infty} \frac{1}{T} \int_0^T f(t)\mathrm{d}t$$

Triple decomposition introduced by *Reynolds and Hussain 1972*

$$\underline{u}(t) = \underbrace{\underbrace{\langle \overline{\underline{u}} \rangle}_{\text{Time average}} + \underbrace{\delta \overline{\underline{u}}(t)}_{\text{temporal fluctuation}}}_{\text{Reynolds average } \overline{\underline{u}}} + \underbrace{\underline{u}'(t)}_{\text{turbulent/rapid fluctuation}}$$

Time averaging of equations

RANS equations

1. We apply the time-average operator $(\cdot)|_0^T \equiv \frac{1}{T}\int_0^T (\cdot)\,\mathrm{d}t$ to the RANS equations
2. At the long term : $(\cdot)|_0^T \underset{T\to+\infty}{\longrightarrow} \langle\cdot\rangle$

- Mass:

$$\text{div}\,(\rho\underline{\overline{u}}) = 0 \longrightarrow \text{div}\left(\rho\,(\underline{\overline{u}})|_0^T\right) = 0$$

- Momentum:

$$\frac{\partial\rho\underline{\overline{u}}}{\partial t} + \underline{\text{div}}\,(\underline{\overline{u}}\otimes\rho\underline{\overline{u}}) = -\underline{\nabla} p - \underline{\text{div}}\left(\rho\underline{\underline{R}}\right)$$

$$\downarrow$$

$$\underline{\text{div}}\,(\langle\underline{\overline{u}}\rangle\otimes\rho\,\langle\underline{\overline{u}}\rangle) = -\underline{\nabla}\,\langle p\rangle - \underline{\text{div}}\left(\rho\left\langle\underline{\underline{R}}\right\rangle + \langle\delta\underline{\overline{u}}\otimes\rho\delta\underline{\overline{u}}\rangle\right)$$

- Transport equation for a passive scalar:

$$\frac{\partial\rho\overline{y}}{\partial t} + \text{div}\,(\overline{y}\rho\underline{\overline{u}}) = -\text{div}\,(\rho\underline{Q}_y)$$

$$\downarrow$$

$$\text{div}\,(\langle\overline{y}\rangle\,\langle\rho\underline{\overline{u}}\rangle) = -\text{div}\,\left(\rho\left\langle\underline{Q}_Y\right\rangle + \langle\rho\delta\overline{y}\delta\underline{\overline{u}}\rangle\right)$$

Physical modelling of the additional contribution

Modelling proposal in case of frozen time-averaged dynamic field

$$-\left\langle \rho \delta \overline{y} \delta \underline{\overline{u}} \right\rangle = C_{\text{low frequency}} \tau \underbrace{\left\langle \delta \underline{\overline{u}} \otimes \rho \delta \underline{\overline{u}} \right\rangle}_{\rho \underline{\underline{\mathcal{R}}}} \cdot \underline{\nabla} \left\langle y \right\rangle$$

with:

- $C_{\text{low frequency}}$ an dimensionless constant
- τ the low frequency fluctuations time scale

$\Rightarrow$ How estimate τ?

From the low-frequency kinetic energy balance, we propose the following estimation:

Low-frequency time scale

$$\tau = \frac{\left\langle \rho \delta \underline{\overline{u}} \cdot \delta \underline{\overline{u}} \right\rangle}{4 \left\langle \mu_T \right\rangle \left\langle \delta \underline{\underline{S}} : \delta \underline{\underline{S}} \right\rangle}$$

Illustration of the triple decomposition methodology

Case description

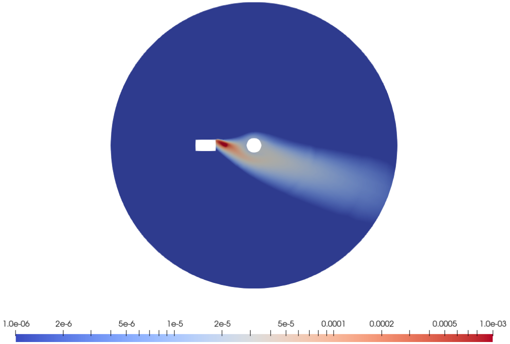
- Boundary Conditions: Monin-Obukhov profiles
  - Direction of incident oscillating meteo velocity

$$\underline{u}_{weather}(z,\, t) = U_{weather}(z) \begin{pmatrix} \sin(\theta(t)) \\ \cos(\theta(t)) \end{pmatrix}$$

with

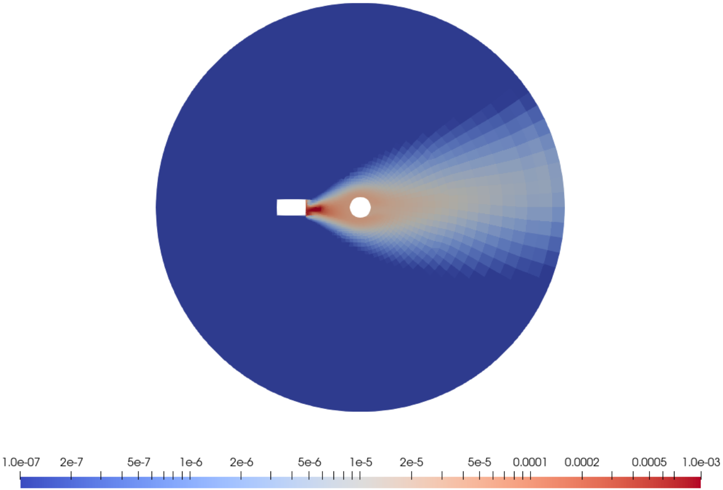
$$\theta(t) = \theta_0 + \delta\theta \sin(\omega t)$$

    - $\theta_0 = 270\,^\circ$ (West wind)
    - $\delta\theta \approx 18\,^\circ$
    - $T = \frac{2\pi}{\omega} = 600\,\mathrm{s}$
- anelastic approximation
- neutral situation ($L_{MO} = +\infty$)
- Turbulence: $k - \epsilon$ model



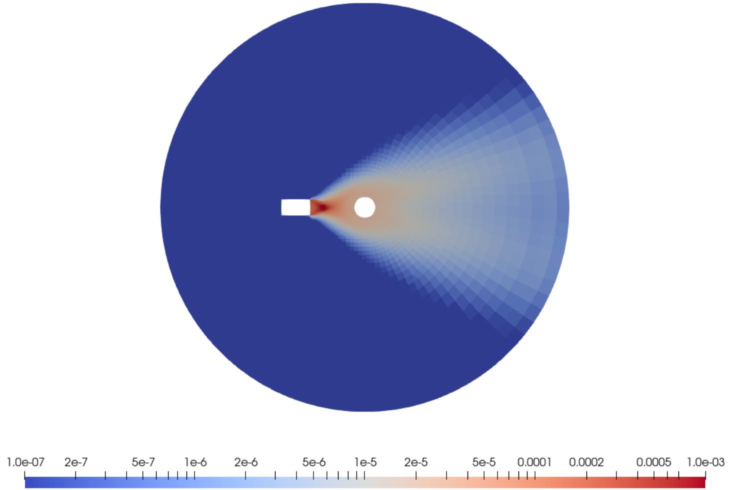
Concentration field with **unsteady** computation of dynamic and emission

$z = 2\,\mathrm{m}$ slice



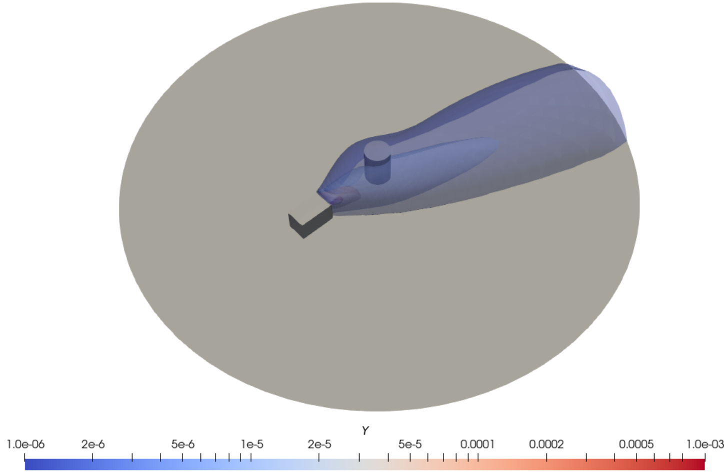
Mean concentration field with **unsteady** computation of dynamic and emission

$z = 2\,\mathrm{m}$ slice, **at the end of the unsteady computation**

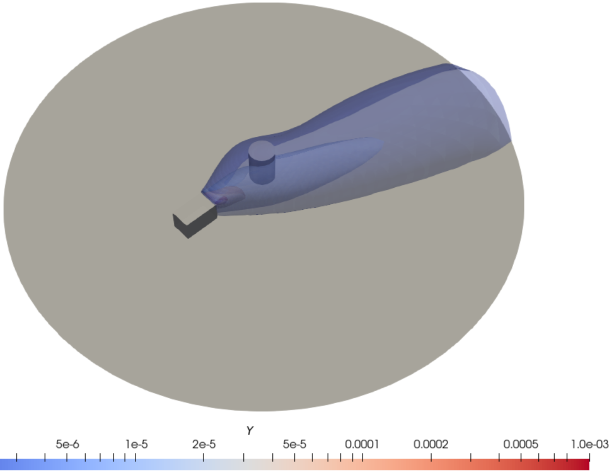


Concentration field with **unsteady** computation of dynamic and emission

isosurfaces

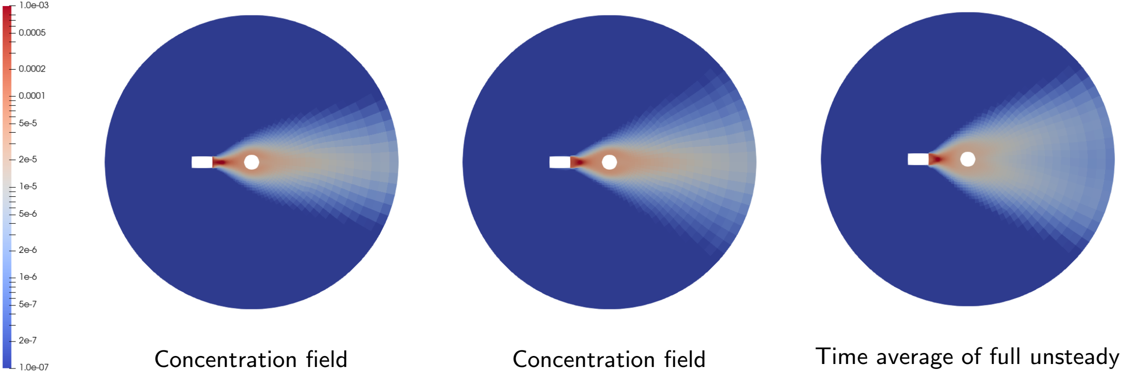


Mean concentration field with **unsteady** computation of dynamic and emission isosurfaces



Dispersion on frozen field dynamic $\langle \underline{u} \rangle$, compared to full unsteady calculation

$z = 2\,\mathrm{m}$ slice



Concentration field without model

Concentration field with model

Time average of full unsteady calculation (Ref)

Low-frequency model on time-averaged frozen dynamic correctly reproduces the plume spread.

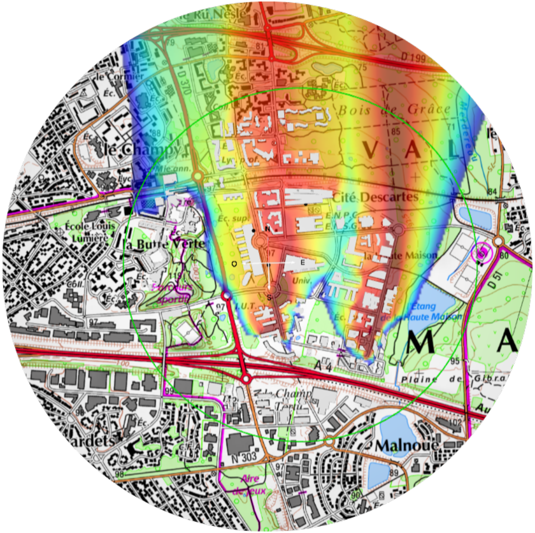
Conclusions and perspectives

Conclusions

- Construction and use of size-optimised wind field.
- Proposal for a diffusion model that qualitatively reconstructs dispersion for a frozen field computation.
- First validation on a toy-model for *outer* low-frequency instationarities.

Perspectives

- Validation for inner instationnarities.
- Validation on SIRTA site.
- Deployment of the methodology on the Cité Descartes atmospheric digital twin.



Thank you for your attention.

Any question?

- Duynkerke, P. G. (1988). "Application of the $E - \varepsilon$ Turbulence Closure Model to the Neutral and Stable Atmospheric Boundary Layer". In: Journal of Atmospheric Sciences.
- Inagaki, Atsushi and Manabu Kanda (2010). "Organized structure of active turbulence over an array of cubes within the logarithmic layer of atmospheric flow". In: Boundary-layer meteorology.
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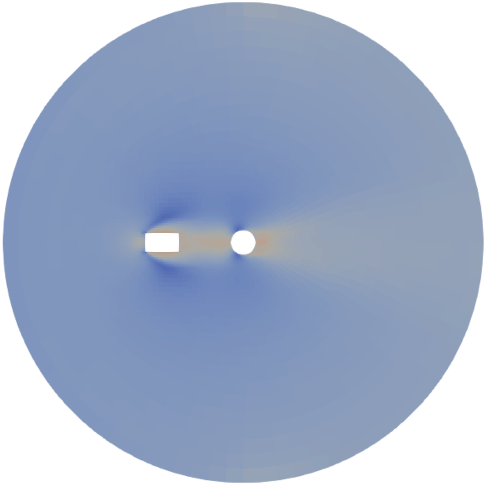
- Reynolds, W. C. and A. K. M. F. Hussain (1972). "The mechanics of an organized wave in turbulent shear flow. Part 3. Theoretical models and comparisons with experiments". In: Journal of Fluid Mec
- Richards, P.J. and S.E. Norris (2011). "Appropriate boundary conditions for computational wind engineering models revisited". In: Journal of Wind Engineering and Industrial Aerodynamics.

Low frequency fluctuations time scale

Slice $z = 2\,\mathrm{m}$



Dry atmosphere model: meteorological fields p_m, ρ_m such that $\underline{\nabla} p_m = \rho_m \underline{g}$ (hydrostatic)

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \text{div}\,(\rho \underline{u}) &= 0, \\
\frac{\partial \rho \underline{u}}{\partial t} + \underline{\text{div}}\,(\underline{u} \otimes \rho \underline{u}) &= -\underline{\nabla} \delta \overline{p} + \underline{\text{div}}\left(\underline{\underline{\tau}} - \rho \underline{\underline{R}}\right) + \delta \rho \underline{g},
\end{aligned}
$$

with

$$
\delta \rho = \rho - \rho_m = -\rho_m \frac{\theta - \theta_m}{\theta} \text{ and } \delta p = p - p_m .
$$

Anelastic approximation: Decomposition of a field as a deviation from the hydrostatic adiabatic atmosphere:

$$
\rho(x, y, z, t) = \underbrace{\rho_0 + \delta \rho_h(z)}_{\rho_a(z)} + \delta^2 \rho(x, y, z, t)
$$

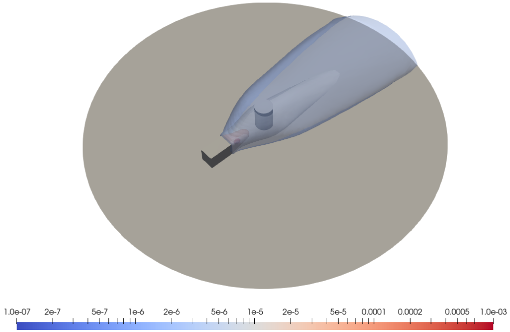
$$
\begin{aligned}
\text{div}\,(\rho_a \underline{u}) &= 0, \\
\frac{\partial \rho_a \underline{u}}{\partial t} + \underline{\text{div}}\,(\underline{u} \otimes \rho_a \underline{u}) &= -\underline{\nabla} \delta \overline{p} + \underline{\text{div}}\left(\underline{\underline{\tau}} - \rho_a \underline{\underline{R}}\right) + \delta \rho \underline{g},
\end{aligned}
$$

where

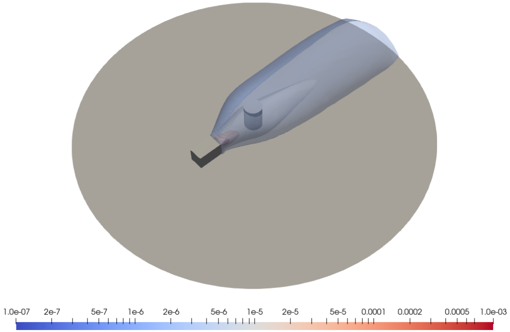
$$
\delta \rho = \rho_a \frac{\theta - \theta_0}{\theta_0} \textbf{ is linear with respect to } \theta - \theta_0
$$

Dispersion on frozen field dynamic $\langle \underline{u} \rangle$, with/without modelling low-frequency fluctuations

isosurfaces



Concentration field with model



Concentration field without model

Dynamic base construction

Discretization of meteorological configurations for a stationary state (or average in time)

3 degrees of freedom

Wind direction

36 directions

Atmospheric stability

L_{MO} (m)	Stab. class
$10 \leq L_{MO} \leq 50$	Very stable
$50 \leq L_{MO} \leq 200$	Stable
$10 \leq L_{MO} \leq 50$	Near stable
$\lvert L_{MO} \rvert \geq 500$	Neutral
$-500 \leq L_{MO} \leq -200$	Near unstable
$-200 \leq L_{MO} \leq -100$	Unstable
$-100 \leq L_{MO} \leq -50$	Very unstable

7 stability classes

Wind velocity

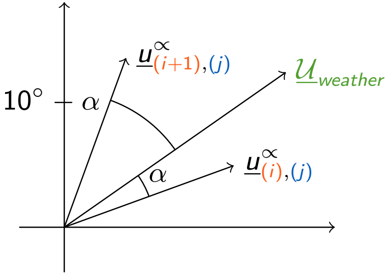
1 single velocity

Valid velocity scaling under anelastic approximation

$36 \times 7 \times 1 = 252$ simulations

$$\underline{u} = \|\underline{\mathcal{U}}_{weather}\| \, f \begin{Bmatrix} \underline{u}^{\propto}_{(i),(j)} & \underline{u}^{\propto}_{(i),(j+1)} \\ \underline{u}^{\propto}_{(i+1),(j)} & \underline{u}^{\propto}_{(i+1),(j+1)} \end{Bmatrix}$$

Example of an interpolation in direction (for a given stability class):



$$\underline{u}_{(j)} = \left[\left(1 - \frac{\alpha}{10^\circ}\right) \underline{\underline{\Omega}}^{\alpha} \underline{u}^{\propto}_{(i),(j)} + \left(\frac{\alpha}{10^\circ}\right) \underline{\underline{\Omega}}^{\alpha-10^\circ} \underline{u}^{\propto}_{(i+1),(j)}\right] ||\underline{\mathcal{U}}_{weather}||$$

with the rotation matrix with angle α (ou $\alpha - 10^\circ$)

$$\underline{\underline{\Omega}}^{\alpha} = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$$